

12. Atoms, Light and their Interaction

In practice, the electromagnetic interaction between atoms and light is manifested in two main ways, coherently or incoherently. The incoherent aspect is seen as damping, noise and radiation, with the principal quantum-mechanical effect being seen as the decay of an excited atom. The coherent aspect arose with the development of the laser as a laboratory tool, and is seen principally in the manipulation of atomic states by the application of appropriately tuned and timed laser pulses. This can be done with great flexibility and precision, and can be used to exert mechanical forces on atoms, leading to the trapping and cooling of atoms.

These two aspects are the extremes. It is never possible to eliminate the incoherent aspects completely, so that a full theory always requires their inclusion, even when the interaction is principally coherent. This is especially true if precise manipulation of the quantum state of an atom is the aim, as in the study of quantum information.

As in the classical case, in quantum mechanics there is a close connection between damping and noise, but in addition, the underlying probabilistic nature of quantum mechanics introduces noise which is purely quantum-mechanical, and not directly connected with damping.

This chapter therefore studies the simplest atomic system—an atom approximated by only two energy levels—interacting with the simplest forms of the electromagnetic field. The two topics are:

- i) *The Decay of an Excited Atom*: Here the atom interacts with an electromagnetic field initially in the vacuum state. We do this because the formalism for quantum noise and damping can become quite elaborate, and the motivation for this formalism can consequently become rather obscure. The radiation of a single photon from a single atom—itself simplified to a system with only two energy levels—provides a useful elementary physical example, introducing the concepts necessary for a full formulation of quantum stochastic processes. A more detailed development of quantum stochastic formalism is presented in the following two chapters, and this is extended and completed in *Book II*.
- ii) *The Manipulation of the Quantum State of an Atom Using a Coherent Optical Field*: Here we omit the quantization of the electromagnetic field, and study

the possible manipulations of the state of a two-level atom that can be executed using coherent optical pulses.

12.1 Interaction with the Quantized Radiation Field

We will use the quantized electromagnetic field as formulated in Sect. 11.1.3, and the main task of this section is to introduce an appropriate formulation of the interaction with a quantized atom.

12.1.1 Hamiltonian and Schrödinger Equation

a) Use of the Schrödinger Picture: For computational purposes the Schrödinger picture is a more appropriate starting point than the Heisenberg picture. This means that the electromagnetic field operators have a mode expansion like those in (11.1.46, 11.1.48), but without the time-dependent exponentials, namely

$$\mathbf{A}_S(\mathbf{x}) = \sum_k \left(\frac{\hbar}{2\omega_k \epsilon_0} \right)^{\frac{1}{2}} \left(a_k \mathbf{u}_k(\mathbf{x}) + a_k^\dagger \mathbf{u}_k^*(\mathbf{x}) \right), \quad (12.1.1)$$

$$\mathbf{E}_S(\mathbf{x}) = i \sum_k \left(\frac{\hbar \omega_k}{2\epsilon_0} \right)^{\frac{1}{2}} \left(a_k \mathbf{u}_k(\mathbf{x}) - a_k^\dagger \mathbf{u}_k^*(\mathbf{x}) \right). \quad (12.1.2)$$

However, in the remainder of this treatment in the Schrödinger picture, we will not explicitly write the subscript S —all operators will implicitly be in the Schrödinger picture.

b) Interaction Hamiltonian: We consider an electron interacting with the quantized electromagnetic field, and bound to a nucleus by an electrostatic field. Using the Coulomb gauge as in Sect. 11.1.3, the Hamiltonian for such a system is

$$H = \frac{(\mathbf{p} - e\mathbf{A}(\mathbf{x}))^2}{2m} + e\phi(\mathbf{x}) + H_{EM}. \quad (12.1.3)$$

In this equation:

- The problem is formulated in the Schrödinger picture, so the vector potential operator has no time dependence.
- The static potential $\phi(\mathbf{x})$ represents the Coulomb potential of the nucleus.
- H_{EM} is the Hamiltonian for the quantized electromagnetic field, as defined in equations (11.1.49) and (11.1.50).

We rewrite the first two parts of (12.1.3) as a Hamiltonian for the bound electron, and a Hamiltonian for the interaction with the quantized electromagnetic field. Thus, we write

$$H \equiv H_0 + V_{\text{Int}} + H_{EM}, \quad (12.1.4)$$

in which

$$H_0 = \frac{\mathbf{p}^2}{2m} + e\phi(\mathbf{x}), \quad (12.1.5)$$

$$V_{\text{Int}} = -\frac{e}{2m}(\mathbf{p} \cdot \mathbf{A}(\mathbf{x}) + \mathbf{A}(\mathbf{x}) \cdot \mathbf{p}) + \frac{e^2}{2m}\mathbf{A}(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}). \quad (12.1.6)$$

Note that the choice of the Coulomb gauge condition (11.1.34) leads to

$$\mathbf{p} \cdot \mathbf{A}(\mathbf{x}) - \mathbf{A}(\mathbf{x}) \cdot \mathbf{p} = -i\hbar\nabla \cdot \mathbf{A}(\mathbf{x}) = 0, \quad (12.1.7)$$

so that the order of factors is not important.

c) Simplifications and Approximations: Formulating the interaction in terms of the vector potential can be awkward, and a reformulation in terms of the electric field and a dipole moment has many advantages, particularly in making approximations. The simplest explanation of the transformation is based on the Lagrangian formulation, in which the electromagnetic interaction of a particle with an electromagnetic field is achieved by the interaction Lagrangian

$$\mathcal{L}_{\text{Int}} = e\dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t). \quad (12.1.8)$$

It is always possible to add a total time derivative to the Lagrangian, so we add such a term so that

$$\mathcal{L}_{\text{Int}} \longrightarrow e\dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t) - \frac{d}{dt}(e\mathbf{x} \cdot \mathbf{A}(\mathbf{x}, t)), \quad (12.1.9)$$

$$= -e\mathbf{x} \cdot \frac{d\mathbf{A}(\mathbf{x}, t)}{dt}, \quad (12.1.10)$$

$$= -e\mathbf{x} \cdot \left(\frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial t} + (\dot{\mathbf{x}} \cdot \nabla) \mathbf{A}(\mathbf{x}, t) \right). \quad (12.1.11)$$

It is at this stage that we can make approximations based on the physics of the situation. The second term in this equation can usually be neglected since:

- The first term is of order of magnitude ωA for a monochromatic field.
- The term ∇A is of order of magnitude $vec A / c\omega$, and if the typical speed of the atom is v , the second term is of order of magnitude v/c smaller than the first term, and is thus almost always negligible.
- We therefore use the approximate form for the interaction Lagrangian

$$\mathcal{L}_{\text{Int}} = e\mathbf{x} \cdot \mathbf{E}(\mathbf{x}, t). \quad (12.1.12)$$

- This form depends on the derivative of field $\mathbf{A}(\mathbf{x}, t)$ and this means that the field canonical momentum variable is no longer $\epsilon_0 \mathbf{E}$, but becomes

$$\mathbf{D}(\mathbf{x}, t) \equiv \epsilon_0 \mathbf{E}(\mathbf{x}, t) - e\mathbf{x}(t) \delta(\mathbf{x} - \mathbf{x}(t)). \quad (12.1.13)$$

The Hamiltonian then becomes

$$\mathcal{H} = H_0 + \int d^3x \left\{ \frac{\mathbf{D}(\mathbf{x}, t)^2}{2\epsilon_0} + \frac{\mathbf{B}(\mathbf{x}, t)^2}{2\mu_0} \right\} - \frac{e\mathbf{x}(t) \cdot \mathbf{D}(\mathbf{x}(t), t)}{\epsilon_0} + \frac{e^2 \mathbf{x}(t)^2 \delta(0)}{\epsilon_0}. \quad (12.1.14)$$

The final term requires interpretation, and we should take the delta function as really being some representation of the size over which the interaction takes place, thus we can reasonably set

$$\delta(0) \longrightarrow \frac{1}{4\pi R^3}, \quad (12.1.15)$$

where R represents the effective size of the interacting system. The term then gives a correction to the electrostatic potential which is a factor $\approx (x(t)/R)^3$ times the Coulomb potential. The correction is an artifact of our neglect of the second term in (12.1.11), and should not be taken as fundamental. We shall neglect it from now on.

d) The Electric Dipole Approximation: It is \mathbf{D} and \mathbf{A} which are basic to the Hamiltonian (12.1.14), but since $\mathbf{D} = \epsilon_0 \mathbf{E}$ except at the position of the atom, we shall not make the distinction, and as our basic Hamiltonian we shall take (12.1.14) with the substitution $\mathbf{D} \longrightarrow \epsilon_0 \mathbf{E}$, which is equivalent to the neglect of the delta function term.

Furthermore, in practice the wavelength of the light is thousands of times larger than the size of an atom, so that the dependence on position of the interaction Hamiltonian is negligible. Assuming then that the atom is located at $\mathbf{x} = 0$, we may write

$$V_{\text{Int}}(t) \rightarrow -e\mathbf{x} \cdot \mathbf{E}(0). \quad (12.1.16)$$

This approximation is known as the *electric dipole approximation*.

e) Atom-Field Hamiltonian in the Electric Dipole Approximation: The Hamiltonian for the full system, after making approximations and simplifications, becomes

$$H = H_{\text{Atom}} + H_{\text{EM}} + H_{\text{Int}}, \quad (12.1.17)$$

with

$$H_{\text{Atom}} = \frac{\mathbf{p}^2}{2m} + e\phi(\mathbf{x}), \quad (12.1.18)$$

$$H_{\text{EM}} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right), \quad (12.1.19)$$

$$H_{\text{Int}} = -\mathbf{d} \cdot \mathbf{E}(0). \quad (12.1.20)$$

Here, we have defined the *electric dipole moment operator*

$$\mathbf{d} \equiv e\mathbf{x}. \quad (12.1.21)$$

12.1.2 The Two-Level Atom Approximation

If the energy eigenstates of the atom are written $|i\rangle$ with energy eigenvalue E_i , then we can write

$$H_{\text{Atom}} = \sum_i E_i |i\rangle\langle i|, \quad (12.1.22)$$

$$ex = \sum_{f,i} \mathbf{d}_{if} |f\rangle\langle i|. \quad (12.1.23)$$

We now make a drastic approximation—we will neglect all but *two* eigenstates, an excited state $|e, E_e\rangle$ and a ground state $|g, E_g\rangle$. This should give a basic understanding of how transitions happen from one state to another.

We can write

$$|e\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |g\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (12.1.24)$$

and consequently in the two-state approximation

$$H_{\text{Atom}} = \begin{pmatrix} E_e & 0 \\ 0 & E_g \end{pmatrix}, \quad (12.1.25)$$

$$ex = \begin{pmatrix} 0 & \mathbf{d}_{eg} \\ \mathbf{d}_{eg}^* & 0 \end{pmatrix}. \quad (12.1.26)$$

We now use the expression (11.1.48) for the electric field operator, and find that (noting that we are in the Schrödinger picture, so that the time dependences in the electromagnetic field operators are omitted) the interaction Hamiltonian becomes

$$H_{\text{Int}} = i\hbar\sigma^- \sum_k \left(a_k^\dagger \kappa_k^* - a_k \bar{\kappa}_k^* \right) - i\hbar\sigma^+ \sum_k \left(a_k \kappa_k - a_k^\dagger \bar{\kappa}_k \right), \quad (12.1.27)$$

and in which

$$\kappa_k \equiv -\sqrt{\frac{\omega_k}{2\hbar\epsilon_0}} \mathbf{d}_{eg} \cdot \mathbf{u}_k(0), \quad \bar{\kappa}_k \equiv -\sqrt{\frac{\omega_k}{2\hbar\epsilon_0}} \mathbf{d}_{eg} \cdot \mathbf{u}_k^*(0). \quad (12.1.28)$$

12.1.3 The Rotating Wave Approximation

A term like $\sigma^+ a_k$ removes a photon from the radiation field, and raises the atom from the ground state to the excited state, and the Hermitian conjugate term $\sigma^- a_k^\dagger$ does the reverse. Provided the energy of the photon is similar to the energy difference between the two atomic eigenstates, this process is *resonant*, and consequently is very significant. On the other hand, the term $\sigma^- a_k$ lowers the atom's energy while also removing a photon from the electromagnetic field, which cannot be resonant, and therefore is not an important process. The *rotating wave approximation* corresponds to omitting terms which cannot be resonant. After making this approximation, the interaction Hamiltonian becomes

$$H_{\text{Int}} = i\hbar \left(\sigma^- \sum_k a_k^\dagger \kappa_k^* - \sigma^+ \sum_k a_k \kappa_k \right). \quad (12.1.29)$$

We can also define the *transition frequency* by

$$\omega = \frac{E_e - E_g}{\hbar}, \quad (12.1.30)$$

then choose the zero of energy so that $E_g = 0$, and write

$$H_{\text{Atom}} \rightarrow \hbar\omega|e\rangle\langle e| = \frac{1}{2}\hbar\omega(1 + \sigma_z). \quad (12.1.31)$$

Thus we arrive at the *Hamiltonian for a two-level atom interacting with the electromagnetic field in the rotating wave approximation*

$$H = \hbar\omega|e\rangle\langle e| + \sum_k \hbar\omega_k a_k^\dagger a_k + i\hbar \left(\sigma^- \sum_k a_k^\dagger \kappa_k^* - \sigma^+ \sum_k a_k \kappa_k \right). \quad (12.1.32)$$

12.1.4 “Stripped-Down” Quantum Electrodynamics

The Hamiltonian (12.1.32), and the various approximations we have introduced in Sect. 12.1.1–Sect. 12.1.3 represent a “stripped-down” version of the quantum electrodynamics originally introduced in Sect. 12.1.1. This description is adequate for most quantum-optical phenomena, and when it is not, it can be usually be extended appropriately. It will be used almost exclusively in the remainder of this book.

12.2 Decay of an Excited Atom

In this section we will show how atomic decay, and hence spectral line broadening, arise from the solution of the Schrödinger equation for the Hamiltonian, in an adaptation of a method formulated by *Weisskopf* and *Wigner* [49] in 1930. Although approximations are made, it will become clear that the irreversibility implicit in atomic decay arises as a result of the continuous energy spectrum of the electromagnetic field rather than the approximations—thus Hamiltonian evolution and irreversibility are not incompatible.

12.2.1 Wavefunction and Initial Condition

We suppose that the initial state consists of no photons in the electromagnetic field, and the atom in the excited state, as illustrated in Fig. 12.1. From this state, the rotating wave Hamiltonian can only create states of the form

$$|g, k\rangle \equiv a_k^\dagger \sigma^- |e, 0\rangle = a_k^\dagger |g, 0\rangle, \quad (12.2.1)$$

where:

- i) $|g, 0\rangle$ is the state with no photons, and the atom in the ground state.

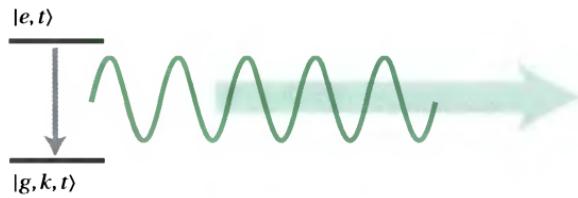


Fig. 12.1. Decay of a two-level atom.

ii) $|e, 0\rangle$ is the state with no photons, and the atom in the excited state.

If we write the time-dependent state of the system in terms of these states as

$$|\Psi, t\rangle = u(e, t)|e, 0\rangle + \sum_k u(g, k, t)|g, k\rangle, \quad (12.2.2)$$

then the Schrödinger equation yields equations of motion for the coefficients in the form

$$i\hbar\dot{u}(e, t) = \hbar\omega u(e, t) - i\hbar\sum_k \kappa_k u(g, k, t), \quad (12.2.3)$$

$$i\hbar\dot{u}(g, k, t) = \hbar\omega_k u(g, k, t) + i\hbar\kappa_k^* u(e, t). \quad (12.2.4)$$

The assumed initial condition of an excited atom and no photons means

$$u(e, 0) = 1, \quad u(g, k, 0) = 0. \quad (12.2.5)$$

a) Solving the Equations: The second equation can be integrated to give

$$u(g, k, t) = e^{-i\omega_k t} u(g, k, 0) + \int_0^t dt' e^{-i\omega_k(t-t')} \kappa_k^* u(e, t'). \quad (12.2.6)$$

The initial condition $u(g, k, 0) = 0$ means that the first term is zero, so we substitute the resulting expression in the first equation to get

$$i\hbar\dot{u}(e, t) = \hbar\omega u(e, t) - i\hbar \int_0^t dt' u(e, t') \left\{ \sum_k |\kappa_k|^2 e^{-i\omega_k(t-t')} \right\}. \quad (12.2.7)$$

This can be simplified if we substitute

$$v(e, t) = u(e, t) e^{i\omega t}, \quad (12.2.8)$$

and it becomes

$$\dot{v}(e, t) = - \int_0^t dt' v(e, t') \left\{ \sum_k |\kappa_k|^2 e^{-i(\omega_k - \omega)(t-t')} \right\}. \quad (12.2.9)$$

b) The Markov Approximation: The function inside the curly brackets

$$\gamma(t-t') \equiv \sum_k |\kappa_k|^2 e^{-i(\omega_k - \omega)(t-t')}, \quad (12.2.10)$$

is central to the understanding of the decay. We can replace the summation by an integral over frequency, and a density of states

$$\sum_k |\kappa_k|^2 \rightarrow \int d\omega_k g(\omega_k) |\kappa(\omega_k)|^2, \quad (12.2.11)$$

where $|\kappa(\omega_k)|^2$ is the average over polarizations of $|\kappa_k|^2$ at the appropriate value of $|\mathbf{k}|$. Thus

$$\gamma(t - t') \rightarrow \int_0^\infty d\omega_k g(\omega_k) |\kappa(\omega_k)|^2 e^{-i(\omega_k - \omega)(t - t')}. \quad (12.2.12)$$

The significant features of this equation are:

- The frequency range of the term $e^{-i(\omega_k - \omega)(t - t')}$ in the integral is $(-\infty, \omega)$.
- ω is itself a very high frequency.
- The coefficient of the exponential is a very smooth function.

These mean that $\gamma(t - t')$ is very small except when $|t - t'|$ is very small. Thus, we can neglect the time variation of $v(e, t')$ inside the integral in (12.2.9), and write

$$\dot{v}(e, t) \approx -v(e, t) \int_0^t \gamma(t - t') dt'. \quad (12.2.13)$$

The approximation that leads to the equation of motion in this form is known as the *Markov approximation*—it enables one to replace the integro-differential equation (12.2.9), which involves $v(e, t')$ for all $t' < t$, by the simpler first-order differential equation (12.2.13). It now remains to evaluate the coefficient on the right-hand side.

c) Significance of the Markov Approximation: The Markov approximation, as it arises here, is the simplest example of how this concept arises in a quantum-mechanical context. It is relevant because there are very different time scales involved. The optical frequencies represent very fast time scales, whereas the decay happens very slowly by comparison. The basic structures of the damping constant and frequency shift which arise here are the same as those found in the more systematic formulations of damping and noise found in the remainder of this book.

d) Evaluation of the Coefficient: Now change variables to $\tau = t - t'$, and evaluate the integral as $\int_0^t d\tau \gamma(\tau)$. In this form, for typical values of t the function $\gamma(\tau)$ is essentially zero when $\tau > t$ so we can set the upper limit of the integral to ∞ with very little error, and the integral can then be written

$$\int_0^\infty \gamma(\tau) d\tau = \lim_{\epsilon \rightarrow 0^+} \int_0^\infty d\tau \int_0^\infty d\omega_k g(\omega_k) |\kappa(\omega_k)|^2 e^{-i(\omega_k - \omega)\tau - \epsilon\tau}. \quad (12.2.14)$$

Here we have inserted a convergence factor $e^{-\epsilon\tau}$, where $\epsilon > 0$ is set equal to zero at the end of the calculation. With this factor inserted, the order of integrals can be interchanged, and we get

$$\int_0^\infty \gamma(\tau) d\tau = \lim_{\epsilon \rightarrow 0} \int_0^\infty d\omega_k \frac{g(\omega_k) |\kappa(\omega_k)|^2}{i(\omega_k - \omega) + \epsilon}, \quad (12.2.15)$$

$$= \lim_{\epsilon \rightarrow 0} \int_0^\infty d\omega_k g(\omega_k) |\kappa(\omega_k)|^2 \left[\frac{\epsilon}{(\omega_k - \omega)^2 + \epsilon^2} - \frac{i(\omega_k - \omega)}{(\omega_k - \omega)^2 + \epsilon^2} \right], \quad (12.2.16)$$

$$\equiv \frac{1}{2} \Gamma + i\delta\omega. \quad (12.2.17)$$

In the limit $\varepsilon \rightarrow 0$, we can write, for any reasonably well-behaved function $f(z)$

$$\int \frac{\varepsilon}{z^2 + \varepsilon^2} f(z) dz \rightarrow \pi f(0), \quad (12.2.18)$$

$$\int \frac{z}{z^2 + \varepsilon^2} f(z) dz \rightarrow P \int \frac{dz f(z)}{z}, \quad (12.2.19)$$

where $P \int$ means the principal value integral. This is often summarized in the formula

$$\int_0^\infty d\tau e^{-iz\tau} = \pi\delta(z) + i\frac{P}{z}. \quad (12.2.20)$$

Exercise 12.1 Principal Value Integral: The principal value integral is defined mathematically by

$$P \int_{-a}^b \frac{dz f(z)}{z} \equiv \lim_{\delta \rightarrow 0+} \left\{ \int_{-a}^{-\delta} \frac{dz f(z)}{z} + \int_{\delta}^b \frac{dz f(z)}{z} \right\}, \quad (12.2.21)$$

where a and b are positive. Show that, when the principal value integral exists, (12.2.19) gives the same result for reasonably well-behaved functions.

e) **Decay Constant and Lineshift:** We can now put together the results we have derived in (12.2.14)–(12.2.21), and thus write (12.2.13) in the form

$$\dot{v}(e, t) = -\left(\frac{1}{2}\Gamma + i\delta\omega\right)v(e, t), \quad (12.2.22)$$

$$\Gamma \equiv 2\pi g(\omega)|\kappa(\omega)|^2, \quad (12.2.23)$$

$$\delta\omega \equiv -iP \int \frac{d\omega_k g(\omega_k)|\kappa(\omega_k)|^2}{\omega - \omega_k}. \quad (12.2.24)$$

Using the initial condition (12.2.5), this leads to the solution

$$u(e, t) = e^{-i(\omega + \delta\omega)t - \Gamma t/2}. \quad (12.2.25)$$

Thus, the interaction with the quantized electromagnetic field leads to an exponential decay of the excited state population $|u(e, t)|^2$, with a lifetime given by $1/\Gamma$. The quantity Γ is called the *decay constant* or the *linewidth*, while $\delta\omega$ is known as the *lineshift*.

The formula for the lineshift as given in (12.2.24) is divergent unless a cutoff is imposed. In our drastically approximated treatment, in which only a single transition is treated, a cutoff would be necessary to eliminate the effect of other transitions, and would thus be a relatively small frequency. A full treatment using relativistic quantum electrodynamics still gives a divergence, which can be remedied using renormalization theory—the resulting shift is known as the *Lamb shift*. The order of magnitude of the shift calculated this way is still much the same as that of the linewidth Γ , and is usually very small.

The decay constant is a much more important parameter, since it leads to qualitatively different behaviour, namely, the decay of excited states and the consequent broadening of the spectral line. Furthermore, the formula (12.2.23) derived for it does not involve the use of cutoffs or renormalization.

12.2.2 Solutions for Atomic Decay and Radiated Field

So far we have studied mainly the state of the atom. The full solutions in this degree of approximation are implicit in the method of solution chosen, and are very illuminating. It is even possible to put these solutions in a form which looks very like that found classically for the radiation from an electric dipole.

a) Full Solution for Field and Atom: Having obtained the solution for $u(e, t)$, we can go back to (12.2.6) to get

$$u(k, g, t) = \kappa_k^* \int_0^t dt' e^{-i\omega_k(t-t')} e^{-(i\omega + \delta\omega + \Gamma/2)t'}, \quad (12.2.26)$$

$$= i\kappa_k^* \left(\frac{e^{-i\omega_k t} - e^{-i(\omega + \delta\omega)t - \Gamma t/2}}{\omega_k - \omega - \delta\omega + i\Gamma/2} \right). \quad (12.2.27)$$

The full solution is now given by (12.2.2), namely

$$|\Psi, t\rangle = u(e, t)|e, 0\rangle + \sum_k u(g, k, t)|g, k\rangle, \quad (12.2.28)$$

with the values of $u(e, t)$ and $u(g, k, t)$ given by (12.2.25, 12.2.27).

b) Entanglement between the Atom and the Electromagnetic Field: The quantum state $|\Psi, t\rangle$ is an *entangled state*. This is a state representing two distinct physical subsystems A and L (in this case the atom and the electromagnetic field) in which it is not possible to write the state as a simple direct product $|a\rangle \otimes |l\rangle$, no matter what bases are chosen for each of the subsystems.

In this case, we *can* write

$$|e, 0\rangle = |e\rangle \otimes |0\rangle, \quad |g, k\rangle = |g\rangle \otimes |k\rangle, \quad (12.2.29)$$

but there is no way of factoring $|\Psi, t\rangle$ itself in the same way into a product of the form $|\text{atom}\rangle \otimes |\text{light}\rangle$. The simplest consequence of this is that if a *photon* is detected, then the *atom* is in the ground state. Even if the photon is detected 100 metres away from the atom, it is *instantly* known that the atom is in the ground state.

Quantum entanglement is the foundation of quantum information and quantum computation, and is treated more extensively in *Book II*.

c) The Radiated Electromagnetic Field: In this state it is clear that

$$\langle \Psi, t | a_k | \Psi, t \rangle = 0, \quad (12.2.30)$$

$$\langle \Psi, t | \sigma^\pm | \Psi, t \rangle = 0, \quad (12.2.31)$$

$$\langle \Psi, t | \sigma_z | \Psi, t \rangle = |u(e, t)|^2 - \sum_k |u(g, k, t)|^2 = 2|u(e, t)|^2 - 1. \quad (12.2.32)$$

Since $\langle \Psi, t | a_k | \Psi, t \rangle = 0$, there is no mean electric field, nor any polarization, which would require non-vanishing $\langle \Psi, t | \sigma^\pm | \Psi, t \rangle$. There is of course a mean square field, and a mean Poynting vector, since these are bilinear in creation and destruction operators.

One would like to get a reasonably simple idea of the propagating radiated electric field, and we can do this by noting that

$$\langle \Psi, t | \sigma^+ a_k | \Psi, t \rangle = u^*(e, t) u(g, k, t) \neq 0. \quad (12.2.33)$$

This is a consequence of the entanglement property noted above; it says that there can be a non-vanishing electromagnetic field if the atom is in the ground state. Making the replacement $\sigma^+ \rightarrow \sigma^-$ in this equation gives zero, showing that it is not possible for there to be a non-vanishing electromagnetic field if the atom is in the excited state.

With these solutions we can now calculate the mean value

$$\langle \mathbf{E}_S^{(+)}(\mathbf{x}, t) \sigma_S^+(t) \rangle = \langle \Psi, t | \mathbf{E}_S^{(+)}(\mathbf{x}) \sigma_S^+ | \Psi, t \rangle. \quad (12.2.34)$$

In this expression, the subscript S emphasizes that we are in the Schrödinger picture, and the operator is not time-dependent. To evaluate this expression we need the expression (12.1.2) and this leads us to evaluate

$$\langle a_k(t) \sigma^+(t) \rangle = \langle a_k^\dagger(t) \sigma^-(t) \rangle^* = \langle \Psi, t | a_k | \Psi, t \rangle = u^*(e, t) u(g, k, t), \quad (12.2.35)$$

$$= \frac{\kappa_k^* e^{-\Gamma t/2}}{\hbar} \left\{ \frac{e^{-i(\omega_k - \omega - \delta\omega)t} - e^{-\Gamma t/2}}{(\omega_k - \omega - \delta\omega) + i\Gamma/2} \right\}. \quad (12.2.36)$$

The mean value we want is then

$$\langle \mathbf{E}^{(+)}(\mathbf{x}, t) \sigma^+(t) \rangle = i \sum_k \left(\frac{\hbar \omega_k}{2\epsilon_0} \right)^{\frac{1}{2}} \langle a_k(t) \sigma^+(t) \rangle \mathbf{u}_k(\mathbf{x}). \quad (12.2.37)$$

The expression can be evaluated, though there is a lot of algebra involved. The final result is

$$\langle \mathbf{E}^{(+)}(\mathbf{x}, t) \sigma^+(t) \rangle = \frac{e^{(i(\omega + \delta\omega) - \Gamma/2)t} \nabla \times (\mathbf{d}_{eg} \times \nabla (\theta(ct - r) e^{(i(\omega + \delta\omega) - \Gamma/2)(r - ct)/c}))}{2(2\pi)^3 \epsilon_0 r}, \quad (12.2.38)$$

where c is the speed of light and $r = |\mathbf{x}|$. The first factor in braces is the time dependence appropriate to σ^+ , while the remaining factor is a propagating damped outgoing wave.

Exercise 12.2 Calculation of the Radiated Field: Verify the result (12.2.38).

12.3 The Two-Level Atom in a Strong Classical Driving Field

Atoms can be manipulated in a wide variety of ways by the application of strong coherent optical fields, for which the quantum nature of the optical field plays a rather unimportant rôle, and thus may be considered to be classical. In this section we will firstly show how transfer from one state to another can be effected, and then discuss the basic principle of an optical trapping potential for a two-level system.

12.3.1 Interaction Hamiltonian

We will develop our treatment in close analogy with that given in Sect. 12.1.1 and Sect. 12.1.2 for the interaction with a quantized electromagnetic field. As in those sections, we start in the Schrödinger picture, but in this case there is no electromagnetic Hamiltonian, and the time dependence of the classical electromagnetic field must be included explicitly in the Schrödinger picture Hamiltonian. Thus, this takes the form

$$H = H_{\text{Atom}} + H_{\text{Int}}, \quad (12.3.1)$$

with

$$H_{\text{Atom}} = \frac{\mathbf{p}^2}{2m} + e\phi(\mathbf{x}), \quad (12.3.2)$$

$$H_{\text{Int}} = -\mathbf{d} \cdot \mathbf{E}(0, t). \quad (12.3.3)$$

Here the electric dipole moment operator is, as previously,

$$\mathbf{d} \equiv e \mathbf{x}. \quad (12.3.4)$$

a) Two-Level Approximation: The interaction with a classical field can then be made with the electric dipole approximation and the two-level system approximation, leading to the Hamiltonian

$$H = \begin{pmatrix} E_e & \mathbf{d}_{eg} \cdot \mathbf{E}(0, t) \\ \mathbf{d}_{eg}^* \cdot \mathbf{E}(0, t) & E_g \end{pmatrix}. \quad (12.3.5)$$

b) Monochromatic Electromagnetic Field: We consider first the case of a strictly monochromatic electromagnetic field, which we introduce in the form (chosen for the convenience of the calculations)

$$\mathbf{d}_{eg} \cdot \mathbf{E}(0, t) = 2i\mathcal{E} \cos(\omega t). \quad (12.3.6)$$

c) Schrödinger Equation in the Interaction Picture: We introduce an interaction picture by writing the wavefunction in the form

$$|\psi, t\rangle = A_e(t)e^{i\omega_e t}|e\rangle + A_g(t)e^{i\omega_g t}|g\rangle = \begin{pmatrix} A_e(t)e^{i\omega_e t} \\ A_g(t)e^{i\omega_g t} \end{pmatrix}, \quad (12.3.7)$$

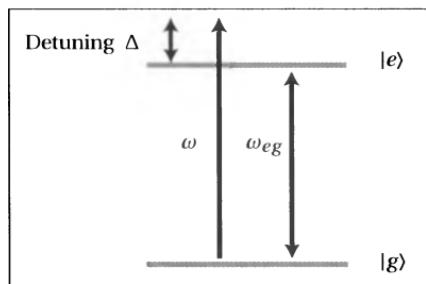


Fig. 12.2. Near-resonant excitation of a two-level system.

and the Schrödinger equation in the interaction picture becomes

$$\dot{A}_e(t) = \frac{2\mathcal{E}}{\hbar} e^{i\omega_{eg}t} \cos \omega t A_g(t), \quad (12.3.8)$$

$$\dot{A}_g(t) = -\frac{2\mathcal{E}^*}{\hbar} e^{-i\omega_{eg}t} \cos \omega t A_e(t). \quad (12.3.9)$$

Here we use the notation

$$\hbar\omega_{eg} \equiv E_e - E_g. \quad (12.3.10)$$

The driven atom and its parameters are illustrated in Fig. 12.2.

12.3.2 Solution of the Schrödinger Equation

a) Rotating Wave Approximation: We can write

$$e^{i\omega_{eg}t} \cos \omega t = \frac{1}{2} e^{i(\omega_{eg}+\omega)t} + \frac{1}{2} e^{i(\omega_{eg}-\omega)t}. \quad (12.3.11)$$

We want to consider the situation in which $\omega_{eg} \approx \omega$, so that the first term oscillates very rapidly with time compared with the second, and we can assume that it averages to zero on the time scale of the solutions of the equations of motion. In this case, the equations simplify to

$$\dot{A}_e(t) = \frac{\mathcal{E}}{\hbar} e^{i(\omega_{eg}-\omega)t} A_g(t), \quad (12.3.12)$$

$$\dot{A}_g(t) = -\frac{\mathcal{E}^*}{\hbar} e^{-i(\omega_{eg}-\omega)t} A_e(t). \quad (12.3.13)$$

b) Rabi Frequency and Detuning: We can simplify the equations by defining:

$$\text{The detuning} \quad \Delta \equiv \omega - \omega_{eg}, \quad (12.3.14)$$

$$\text{The Rabi frequency} \quad \Omega_R \equiv \left| \frac{2\mathcal{E}}{\hbar} \right| = \left| \frac{\mathbf{d}_{eg} \cdot \mathbf{E}}{\hbar} \right|, \quad (12.3.15)$$

$$\text{The phase of } \mathcal{E} \text{ by} \quad \mathcal{E} \equiv |\mathcal{E}| e^{i\phi}. \quad (12.3.16)$$

c) Rabi Hamiltonian: We can remove the explicit time dependence of the coefficients by writing

$$a_e(t) \equiv A_e(t)e^{i(\Delta t - \lambda)}, \quad a_g(t) \equiv A_g(t)e^{i\lambda}, \quad \lambda = \phi/2 - \pi/4, \quad (12.3.17)$$

which leaves the equations in the *Rabi Hamiltonian* form

$$i\hbar \frac{d}{dt} \begin{pmatrix} a_e(t) \\ a_g(t) \end{pmatrix} = H_{\text{Rabi}}(\Omega_R, \Delta) \begin{pmatrix} a_e(t) \\ a_g(t) \end{pmatrix}, \quad (12.3.18)$$

in which

$$H_{\text{Rabi}}(\Omega_R, \Delta) \equiv \hbar \begin{pmatrix} -\Delta & -\frac{1}{2}\Omega_R \\ -\frac{1}{2}\Omega_R & 0 \end{pmatrix}. \quad (12.3.19)$$

12.3.3 Optical Pulses

Using pulsed laser fields, it is possible to manipulate the quantum state of a two-level system, and this forms the basis of concept of *quantum state engineering*. In this case, the equation of motion remains the same as (12.3.18), but the Rabi frequency becomes $\Omega_R(t)$, a time-dependent quantity.

The most important special case of a pulse shape is the *rectangular pulse*

$$\mathcal{E}(t) = \begin{cases} \mathcal{E}, & \text{for } 0 \leq t \leq T, \\ 0, & \text{otherwise.} \end{cases} \quad (12.3.20)$$

Here the step function must be understood as being “slow” on the optical time scale that is, the step function is an idealization of the turning on and off of an optical field, both of which take place over many optical cycles.

a) Validity of the Rotating Wave Approximation: The condition for the off resonant terms to be negligible requires that all time dependences retained and of interest must be on a slow time scale. This means that

$$\Omega_R \ll \omega \approx \omega_{eg}, \quad (12.3.21)$$

$$|\Delta| \ll \omega \approx \omega_{eg}, \quad (12.3.22)$$

and as well that $\mathcal{E}(t)$ be slowly varying on the optical time scale, which requires

$$\left| \frac{1}{\mathcal{E}(t)} \frac{d\mathcal{E}(t)}{dt} \right| \ll \omega. \quad (12.3.23)$$

This means that a “instantaneous” turn on of a square pulse as in (12.3.20) has to be interpreted as being slow on the optical time scale, but fast on the time scales given by Ω_R and Δ .

Under these conditions, the coefficients $a_e(t)$ and $a_g(t)$ are also slowly varying on the optical time scale.

b) On-Resonance Rabi Oscillations: For $\Delta = 0$ we have

$$i \frac{d}{dt} \begin{pmatrix} a_e \\ a_g \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2}\Omega_R(t) \\ -\frac{1}{2}\Omega_R(t) & 0 \end{pmatrix} \begin{pmatrix} a_e \\ a_g \end{pmatrix}. \quad (12.3.24)$$

These equations can be solved exactly by writing them in terms of the total angle given by the time integral of the Rabi frequency. Thus we introduce the variable

$$\tau(t) \equiv \int_{-\infty}^t \Omega_R(t) dt, \quad (12.3.25)$$

as a new variable instead of time, and we then solve the equation exactly in the form

$$\begin{pmatrix} a_e(t) \\ a_g(t) \end{pmatrix} = U_t \begin{pmatrix} a_e(-\infty) \\ a_g(-\infty) \end{pmatrix}, \quad (12.3.26)$$

$$\text{where } U_t \equiv \begin{pmatrix} \cos \frac{1}{2}\tau(t) & -i \sin \frac{1}{2}\tau(t) \\ -i \sin \frac{1}{2}\tau(t) & \cos \frac{1}{2}\tau(t) \end{pmatrix}. \quad (12.3.27)$$

The probability of being in the excited state, having initially been in the ground state, oscillates, a phenomenon called *Rabi oscillations*:

$$P_{e \leftarrow g}(t) = \sin^2 \frac{1}{2}\tau(t) = \frac{1}{2}(1 - \cos \tau(t)). \quad (12.3.28)$$

c) Particular Pulses:

i) A π -pulse is defined by a choice of the function $\mathcal{E}(t)$ so that the total angle generated from beginning to the end of the pulse is π , that is

$$\tau^\pi(\infty) = \int_{-\infty}^{\infty} \Omega_R^\pi(t) dt = \pi. \quad (12.3.29)$$

The effect of this is to invert the two-level system, so that

$$U_\infty^\pi = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}. \quad (12.3.30)$$

ii) A 2π -pulse is similarly defined by a different choice of the function $\mathcal{E}(t)$ so that the total angle is 2π , that is

$$\tau^{2\pi}(\infty) = \int_{-\infty}^{\infty} \Omega_R^{2\pi}(t) dt = 2\pi. \quad (12.3.31)$$

This pulse inverts the two-level system twice, thus returning it to its ground state,

$$U_\infty^{2\pi} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad (12.3.32)$$

but with a negative sign for the amplitudes, because a rotation of a spin half system by 2π induces a sign change.

iii) A pulse can be chosen to give any rotation angle required. By allowing non-resonant pulses as well, we can also manipulate the relative phase of the excited and ground state amplitudes.

12.3.4 Effective Potential on a Ground State Atom

We consider the case where $A_g(0) = 1$, and $A_e(0) = 0$, that is an atom initially in its ground state. In this case we integrate (12.3.12) and substitute this into (12.3.13) to get

$$\dot{A}_g(t) = -\frac{\Omega_R^2}{4} \int_0^t dt' e^{i\Delta(t-t')} A_g(t') - \frac{\mathcal{E}}{\hbar} e^{i\Delta t} A_e(0). \quad (12.3.33)$$

Consider the case where $|\Omega_R|^2$ is sufficiently small that $A_g(t)$ varies slowly compared to the oscillating exponential; in this case:

- i) The second term will oscillate very rapidly on this time scale, and average to zero—therefore we can omit this term.
- ii) Because $A_g(t)$ varies slowly, we can write

$$\dot{A}_g(t) \approx -\frac{\Omega_R^2}{4} A_g(t) \int_0^t dt' e^{i\Delta(t-t')}, \quad (12.3.34)$$

$$= -i \frac{\Omega_R^2}{4} A_g(t) \frac{1 - e^{i\Delta t}}{\Delta}. \quad (12.3.35)$$

- a) **The Optical Potential:** As above, on the time scale in which $A_g(t)$ changes, we can neglect the rapidly varying exponential term, to get a simple equation for the ground state amplitude

$$i\hbar \dot{A}_g(t) \approx \frac{\hbar \Omega_R^2}{4\Delta} A_g(t). \quad (12.3.36)$$

This is a very simple kind of Schrödinger equation for the ground state atom under the influence of an off-resonance light field, in which there is effectively an *optical potential* defined by

$$V_{\text{opt}} = \frac{\hbar \Omega_R^2}{4\Delta}. \quad (12.3.37)$$



Fig. 12.3. Left: Schematic of an optical trap created by a tightly focused laser beam; Right: Individual atoms can be trapped on demand in a FORT [50], and the image shows a single ^{85}Rb atom trapped in a FORT in the laboratory of Dr Mikkel F. Andersen at the University of Otago (June 2010), where the technique was developed. (Image kindly supplied by Dr Andersen.)

b) Properties of the Optical Potential:

- i) The result requires that $\Delta \gg \Omega_R$, since the time rate of change of A_g must be very much slower than that corresponding to Δ . From (12.3.37), this requires that $\Omega_R^2/\Delta \ll \Delta$, giving the result.
- ii) *Red detuning* means that $\omega < \omega_{eg}$, that is the driving field has a frequency less than the transition frequency. In this case $V_{\text{opt}} < 0$, and the potential attracts.
- iii) *Blue detuning* means that $\omega > \omega_{eg}$, that is the driving field has a frequency greater than the transition frequency. In this case $V_{\text{opt}} > 0$, and the potential repels.

c) Optical Trapping—the FORT: The acronym FORT means the *Far Off Resonance Trap*. If we take a spatially dependent optical field, in which the spatial dependence of the field is on a spatial scale much larger than that of the atomic wavefunction, the Rabi frequency becomes spatially dependent $\Omega_R(\mathbf{x})$, and the optical potential also becomes spatially dependent. The energies involved are in practice quite small, so that the potential is quite weak, but still strong enough to trap atoms at microKelvin temperatures—see Fig. 12.3.

 **Exercise 12.3 Direct Derivation from the Hamiltonian:** Find the energy eigenvalues of the Hamiltonian matrix (12.3.19), and show that when $\Delta \gg \Omega_R$, they give the optical potential. What else can you deduce from these eigenvalues?

12.4 Interaction of a Two-Level Atom with a Single Mode

By using an optical cavity the interaction with a particular mode of the cavity can be so enhanced that the other modes can be neglected completely, leaving the *Jaynes–Cummings* [51] Hamiltonian

$$H = H_0 + H_1, \quad (12.4.1)$$

$$H_0 = \frac{1}{2}\hbar\omega\sigma_z + \hbar\omega a^\dagger a, \quad (12.4.2)$$

$$H_1 = \hbar g(a\sigma^+ + a^\dagger\sigma^-). \quad (12.4.3)$$

Notice that $[H_0, H_1] = 0$, so that we can move to the interaction picture without changing the interaction Hamiltonian.

If the initial state of the system is $|e, n\rangle$, a state of n photons with the atom excited, the only other state connected is $|g, n+1\rangle$. Thus, the state can be written

$$|\Psi, t\rangle = u(e, t)|e, n\rangle + u(g, t)|g, n+1\rangle, \quad (12.4.4)$$

$$\text{with } u(e, 0) = 1, \quad u(g, 0) = 0. \quad (12.4.5)$$

and the equations of motion in the interaction picture are

$$i\dot{u}(e, t) = g\sqrt{n+1}u(g, t), \quad (12.4.6)$$

$$i\dot{u}(g, t) = g\sqrt{n+1}u(e, t). \quad (12.4.7)$$

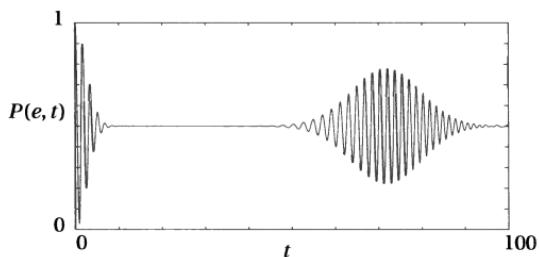


Fig. 12.4. Quantum revivals in the occupation probability of the excited state as given by (12.4.13).

Setting $\Omega_n = g\sqrt{n+1}$, these equations have the solution

$$u(e, t) = \cos(\Omega_n t), \quad (12.4.8)$$

$$u(g, t) = -i \sin(\Omega_n t). \quad (12.4.9)$$

The system thus oscillates back and forth from excited to ground state of the atom, with the energy moving back and forth from the field to the atom. The probability of finding the atom in the excited state (and with n photons) is

$$P(e, t) = \cos^2 \Omega_n t. \quad (12.4.10)$$

12.4.1 Quantum Collapses and Revivals

Suppose we put the field in an initial coherent state, and the atom in the excited state

$$|\Psi, 0\rangle = |e, \alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |e, n\rangle, \quad (12.4.11)$$

then this state evolves into

$$|\Psi, t\rangle = e^{-|\alpha|^2} \sum_n \frac{\alpha^n}{\sqrt{n!}} \{ \cos \Omega_n t |e, n\rangle + \sin \Omega_n t |g, n\rangle \}. \quad (12.4.12)$$

The probability of occupation of the excited state is

$$P(e, t) = e^{-|\alpha|^2} \sum_n \frac{|\alpha|^n}{n!} \cos^2 \Omega_n t. \quad (12.4.13)$$

The different frequencies are incommensurate with each other, and soon get out of phase, so the probability of the excited state decays initially. However, since there are only a finite number which are effectively occupied, eventually the important ones can get in phase again, and the probability has a *quantum revival*, as illustrated in Fig. 12.4. The terminology “quantum revival” reflects the fact that this behaviour is a direct consequence of quantization.